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APPLICATION NO.	FILING DATE	FIRST NAMED INVENTOR	ATTORNEY DOCKET NO.	CONFIRMATION NO.
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10/598,931

09/14/2006

Marcus A. Neumann

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20575

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07/09/2010

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EXAMINER

DEJONG, ERIC S

ART UNIT

PAPER NUMBER

1631

NOTIFICATION DATE

DELIVERY MODE

07/09/2010

ELECTRONIC

Please find below and/or attached an Office communication concerning this application or proceeding.

The time period for reply, if any, is set in the attached communication.

Notice of the Office communication was sent electronically on above-indicated "Notification Date" to the following e-mail address(es):

docketing@techlaw.com

Office Action Summary	Application No.	Applicant(s)	
	10/598,931	NEUMANN, MARCUS A.	
	Examiner	Art Unit	
	ERIC S. DEJONG	1631	

-- The MAILING DATE of this communication appears on the cover sheet with the correspondence address --

Period for Reply

A SHORTENED STATUTORY PERIOD FOR REPLY IS SET TO EXPIRE 3 MONTH(S) OR THIRTY (30) DAYS, WHICHEVER IS LONGER, FROM THE MAILING DATE OF THIS COMMUNICATION.

- Extensions of time may be available under the provisions of 37 CFR 1.136(a). In no event, however, may a reply be timely filed after SIX (6) MONTHS from the mailing date of this communication.
- If NO period for reply is specified above, the maximum statutory period will apply and will expire SIX (6) MONTHS from the mailing date of this communication.
- Failure to reply within the set or extended period for reply will, by statute, cause the application to become ABANDONED (35 U.S.C. § 133). Any reply received by the Office later than three months after the mailing date of this communication, even if timely filed, may reduce any earned patent term adjustment. See 37 CFR 1.704(b).

Status

- 1) ☒ Responsive to communication(s) filed on 16 April 2010.
- 2a) ☐ This action is **FINAL**. 2b) ☒ This action is non-final.
- 3) ☐ Since this application is in condition for allowance except for formal matters, prosecution as to the merits is closed in accordance with the practice under *Ex parte Quayle*, 1935 C.D. 11, 453 O.G. 213.

Disposition of Claims

- 4) ☒ Claim(s) 1-18 is/are pending in the application.
- 4a) Of the above claim(s) 10-14, 17 and 18 is/are withdrawn from consideration.
- 5) ☐ Claim(s) _____ is/are allowed.
- 6) ☒ Claim(s) 1-9, 15 and 16 is/are rejected.
- 7) ☐ Claim(s) _____ is/are objected to.
- 8) ☐ Claim(s) _____ are subject to restriction and/or election requirement.

Application Papers

- 9) ☐ The specification is objected to by the Examiner.
- 10) ☒ The drawing(s) filed on 14 September 2006 is/are: a) ☒ accepted or b) ☐ objected to by the Examiner.
Applicant may not request that any objection to the drawing(s) be held in abeyance. See 37 CFR 1.85(a).
Replacement drawing sheet(s) including the correction is required if the drawing(s) is objected to. See 37 CFR 1.121(d).
- 11) ☐ The oath or declaration is objected to by the Examiner. Note the attached Office Action or form PTO-152.

Priority under 35 U.S.C. § 119

- 12) ☒ Acknowledgment is made of a claim for foreign priority under 35 U.S.C. § 119(a)-(d) or (f).
- a) ☒ All b) ☐ Some * c) ☐ None of:
1. ☒ Certified copies of the priority documents have been received.
2. ☐ Certified copies of the priority documents have been received in Application No. _____.
3. ☐ Copies of the certified copies of the priority documents have been received in this National Stage application from the International Bureau (PCT Rule 17.2(a)).

* See the attached detailed Office action for a list of the certified copies not received.

Attachment(s)

- | | |
|--|---|
| 1) <input checked="" type="checkbox"/> Notice of References Cited (PTO-892) | 4) <input type="checkbox"/> Interview Summary (PTO-413) |
| 2) <input type="checkbox"/> Notice of Draftsperson's Patent Drawing Review (PTO-948) | Paper No(s)/Mail Date. _____ |
| 3) <input checked="" type="checkbox"/> Information Disclosure Statement(s) (PTO/SB/08) | 5) <input type="checkbox"/> Notice of Informal Patent Application |
| Paper No(s)/Mail Date <u>09/14/2006</u> . | 6) <input type="checkbox"/> Other: _____ |

DETAILED OFFICE ACTION

Applicants response filed 04/16/2010 is acknowledged.

Election/Restrictions

Applicant's election without traverse of Group I (claims 1-9, 15, and 16) in the reply filed on 04/16/2010 is acknowledged.

Claims 1-18 are pending. Claims 10-14, 17, and 18 are withdrawn from further consideration pursuant to 37 CFR 1.142(b) as being drawn to a nonelected of Group II, there being no allowable generic or linking claim. Election was made **without** traverse in the reply filed on 04/16/2010.

Claims 1-9, 15, and 16 are currently under examination.

Information Disclosure Statement

The information disclosure statement (IDS) submitted on 09/14/2006 has been considered by the examiner.

Claim Rejections - 35 USC § 101

35 U.S.C. 101 reads as follows:

Whoever invents or discovers any new and useful process, machine, manufacture, or composition of matter, or any new and useful improvement thereof, may obtain a patent therefor, subject to the conditions and requirements of this title.

Claims 1-9, 15, and 16 are rejected under 35 U.S.C. 101 because the claimed invention is directed to non-statutory subject matter.

The instant claims are drawn to a method calculating van der Waals parameters from a simulated crystal structure derived from density functional theory (DFT). The recited steps within the claims themselves do not act on nor transform any particular article into a different state or thing. Further, the recited steps do not involve any machine or apparatus. Rather, the instant claims recite the generalized, abstract computational steps involved in performing a best fit calculation for van der Waals parameters with respect to a given crystal structure. Such amounts only to a series of abstract steps directed toward performing a particular calculation limited to the field of molecular structure determination. For these reasons, the claims encompass an abstract idea comprising mental steps and, therefore, is directed to non-statutory subject matter.

Claim Rejections - 35 USC § 103

The following is a quotation of 35 U.S.C. 103(a) which forms the basis for all obviousness rejections set forth in this Office action:

(a) A patent may not be obtained though the invention is not identically disclosed or described as set forth in section 102 of this title, if the differences between the subject matter sought to be patented and the prior art are such that the subject matter as a whole would have been obvious at the time the invention was made to a person having ordinary skill in the art to which said subject matter pertains. Patentability shall not be negated by the manner in which the invention was made.

Claims 1-9, 15, and 16 are rejected under 35 U.S.C. 103(a) as being unpatentable over Cornell et al. (J. Chem. Soc., 1995).

The instant claims are drawn to a method for the accurate determination of van der Waals parameters for high precision determination of crystal structures and/or energies. The recited process comprises the steps of providing reference data containing reference data and a simulated crystal structure, defining a deviation function quantifying a deviation between said reference data and simulated crystal structure, fitting at least one parameter of a van der Waals potential term so as to minimize the deviation function, and obtaining the accurate van der Waals parameters from the best fit.

Cornell et al. teaches that the application of computer-based models using analytical potential energy functions has proven to be a powerful tool for studying molecules of biochemical and organic chemical interest. Cornell et al. further teaches that given their importance, much effort has gone into consideration of both the functional form and the parameters that must be established in order to apply such analytical potential energy functions. See page 5179, col. 1 in its entirety. Cornell et al. expressly teaches the application of an analytical approach to fitting energy parameters used in modeling molecules to empirical results available through experimentation. See page 5179, col. 2, line 1 through page 5181, col. 2, line 18. Further, Cornell et al. provide the algorithm arrived at by the above described approach, a model described as "minimalist" in its functional form, that is to be applied in modeling of molecular structures. See page 5181, col. 2, lines 20-22. It is further noted that the algorithm provided accounts for the van der Waals parameters as instantly claimed.

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While Cornell et al. teaches defining a deviation function quantifying a deviation between reference and simulated crystal structure data, fitting at least one parameter of a van der Waals potential term so as to minimize the deviation function, and obtaining the accurate van der Waals parameters from the best fit, Cornell et al. does not expressly teach the numerical simulation of a crystal structure based on density functional theory. However, Cornell et al. does provide ample discussion regarding the use of the disclosed procedures in relation to structure determination and analysis of biochemical and biological molecules, which encompasses the use general use of crystal structures as commonly known and applied in this art. Upon review, the instant disclosure does not assert nor support that applicants art the first to use or invention density functional theory as it applied to X-ray crystallography and the determination of high resolution molecular structure. As such, The difference between the instant claims and that of the prior art rests only on the use of crystal structures derived using density functional theory, a technique which already known and utilized in the art. Absent evidence to the contrary, one of skill in the art would be motivated to rely upon the best available crystal structures that the prior art can provide. In the instant case, the selection of crystal structures realized using density functional theory (a technique already known and utilized in the art) would require only a common sense desire to use the best available information in a modeling method. Therefore it would have been obvious at the time the invention was made to a person having ordinary skill in the art to which said subject matter to rely upon crystal structures derived using density functional theory.

Conclusion

Any inquiry concerning this communication or earlier communications from the examiner should be directed to ERIC S. DEJONG whose telephone number is (571)272-6099. The examiner can normally be reached on 8:30AM-5:00PM.

If attempts to reach the examiner by telephone are unsuccessful, the examiner's supervisor, Marjorie Moran can be reached on (571) 272-0720. The fax phone number for the organization where this application or proceeding is assigned is 571-273-8300.

Information regarding the status of an application may be obtained from the Patent Application Information Retrieval (PAIR) system. Status information for published applications may be obtained from either Private PAIR or Public PAIR. Status information for unpublished applications is available through Private PAIR only. For more information about the PAIR system, see <http://pair-direct.uspto.gov>. Should you have questions on access to the Private PAIR system, contact the Electronic Business Center (EBC) at 866-217-9197 (toll-free). If you would like assistance from a USPTO Customer Service Representative or access to the automated information system, call 800-786-9199 (IN USA OR CANADA) or 571-272-1000.

/ERIC S. DEJONG/
Primary Examiner, Art Unit 1631